List of Contents

NUMBER 1

	i	Softstrip® data strip containing the table of contents for this issue
L. L. Miller and **R. A. Jacobson**	1	A self-consistent semi-empirical absorption correction technique
Zong Jie Liu and **Roland Van Rapenbusch**	5	A fast system for the best matching of two sets of atomic coordinates
Pierre Dufour, Martine Dumont, Vincent Chabart and **Jacques Lion**	25	Monte-Carlo simulation of surface reactions (revisited)
Marco S. Caceci	33	A simple, performant diode array spectrophotometer
Marius D'Amboise and **Benoit Lagarde**	39	Factor analysis using column cross-validation
Michael G. Martl and **Klaus Hummel**	45	A simulation program for investigating substitution in polyalkenylenes coupled with double bond shifts
Gy. Dömötör and **M. I. Bán**	53	Dynamic level-shifting
Marvin Bishop and **Michael Csontos Jr**	59	Polymer dynamics movies generated by program spacefil
C. Wade Sheen and **Randy W. Snyder**	61	An automated integration routine for FT-IR spectrometers
Applications		
A. C. J. Kuiper, R. E. F. Einerhand and **W. Visscher**	69	Computer controlled testing of batteries
Denis K. C. Leung and **R. S. Tse**	75	Data acquisition with the IBM PC/XT/AT family—I. A medium speed system for the XT or AT
S. Q. Lew and **R. S. Tse**	89	Microcomputer automation of coulometric titration
Letter to the Editor		
Yoshitaka Beppu	101	New version of NAMOD (Nagoya Molecular Display) program
Errata	103	

NUMBER 2

A Selection of Papers Presented
at

THE WORKSHOP ON MOLECULAR MECHANICS AND MOLECULAR DYNAMICS

Carlos F. Bunge	105	Malleable software for *ab-initio* quantum chemistry
DeLos F. DeTar	111	Modular molecular mechanics programs and transportable force fields—a partly implemented proposal
Ramon Garduño-Juarez and **Elsa Ocampo-Garcia**	117	Conformational studies by molecular mechanics and molecular orbital methods on the antiamoebic drug 1-(4-imidazolylsulfonyl)-4-phenylimidazole
Markus Breuer and **Gerhard Hägele**	123	Determination of approximate force field parameters
Reginald C. Haines	129	Computer graphics for processing chemical substance information
Joyce J. Kaufman, Szczepan Roszak, P. C. Hariharan and **Phillip B. Keegstra**	141	A new computational strategy for *ab-initio* MRD–CI calculations for breaking a chemical bond in a molecule in a crystal or other solid environment
E. K. Davies and **N. W. Murrall**	149	How accurate does a force field need to be?
James J. P. Stewart	157	Example of the advantage of the BFGS geometry optimizer over the DFP
Carl Trindle	159	Viewing the molecular display: hints from the artificial intelligence of vision
	I	Softstrip® data strip containing the table of contents for this issue

NUMBER 3

	i	Softstrip® data strip containing the table of contents for this issue
DeLos F. DeTar	iii	Editorial
Thomas M. Zamis, Lawrence J. Parkhurst and **Gordon A. Gallup**	165	A matrix series method for the integration of rate equations in a reaction network. An alternative to Runge–Kutta methods
Michael Albin and **Harry B. Gray**	173	Multi-variant kinetic analyses on a microcomputer
R. E. Hoffman and **G. C. Levy**	179	Optimization of NMR data processing with coarse-grain parallel computers

Peter C. Kahn	185	Defining the axis of a helix
Peter C. Kahn	191	Simple methods for computing the least squares line in three dimensions
J. M. Sevilla, M. Dominguez, F. Garcia-Blanco and **M. Blazquez**	197	Resolution of absorption spectra
Annik Vivier Bunge, Carlos F. Bunge, Rocio Jáuregui and **Gerardo Cisneros**	201	Symmetry-eigenfunctions for many-electron atoms and molecules: a unified and friendly approach for frontier research and student training
Rocio Jáuregui, Carlos F. Bunge, Annik Vivier Bunge and **Gerardo Cisneros**	223	Angular momentum eigenfunctions for many-electron calculations
Annik Vivier Bunge, Carlos F. Bunge, Rocio Jáuregui and **Gerardo Cisneros**	239	Spin eigenfunctions for many-electron calculations
Gerardo Cisneros, Rocio Jáuregui, Carlos F. Bunge and **Annik Vivier Bunge**	255	Molecular symmetry eigenfunctions for many-electron calculations
Carlos F. Bunge	271	Schmidt orthonormalization of a basis expressible both as linear combinations and as projections of orthonormal primitive functions
Carlos F. Bunge, Rocio Jáuregui and **Gerardo Cisneros**	277	Writing friendly programs in modular form
Kim H. Chow and **Melvin B. Comisarow**	291	Magnitude-Lorentzian interpolation of discrete, absorption-mode Fourier transform spectra
Book Reviews		
DeLos F. DeTar	297	Computational Chemistry, by M. D. Johnston Jr
DeLos F. DeTar	297	Expert Systems 85. Edited by Martin Merry
DeLos F. DeTar	297	Numerical Recipes, by William H. Press, Brian P. Flannery, Saul A. Teukolsky and William T. Vetterling
DeLos F. DeTar	298	Computation of Solution Equilibria, by M. Melhoun, J. Havel and E. Högfeldt

NUMBER 4

i Softstrip® data strip containing the table of contents for this issue

I. B. C. Matheson	299	Robust estimation of parameters: a simple modification to all non-linear fitting algorithms to convert from minimizing the sum of squares of deviations to minimizing the sum of the absolute deviations
Zdeněk Slanina	305	A program for determination of composition and thermodynamics of the ideal gas-phase equilibrium isomeric mixtures
J. C. Sauniere, T. P. Lybrand, J. A. McCammon and **L. D. Pyle**	313	Polarizable water models: vectorization of energy calculations on the CYBER 205
W. R. Creasy and **J. T. Brenna**	319	Interface between a Nicolet FTMS/2000 and a Quantel Nd:YAG laser using an IBM PC-AT
V. Gadjokov and **H. Mihailova**	325	KATCOM: a microcomputer program for the computation of stability constants from potentiometric titration data
David C. Feller, Ernest F. Delmoe and **S. Scott Zimmerman**	337	Conformational energy analysis of peptides using microcomputers: description of PepCAD™ and analysis of *N*-formyl-*N'*-methylalanineamide
Concetta De Stefano, Pietro Princi, Carmelo Rigano and **Silvio Sammartano**	343	The calculation of equilibrium concentrations. ES4EC1: a FORTRAN program for computing distribution diagrams and titration curves
Zdeněk Slanina	361	A procedure for the evaluation of the reduced moment of inertia for internal rotation
Charles Brochu and **Emilien Pelletier**	367	A microcomputer program for the analysis of gas chromatographic data
I. B. C. Matheson	385	The non-equivalence of Padé–Laplace and non-linear least squares data fitting: a Padé–Laplace bias towards slower processes
François-Xavier Bon and **Roland van Rapenbusch**	387	"CHOODRAW"—an interactive molecular graphics program (PC/XT/AT) to display small molecules complexed with protein fragments selected from the protein data bank